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2000 J. Phys. A: Math. Gen. 33 6981

(http://iopscience.iop.org/0305-4470/33/39/312)

J. Phys. A: Math. Gen. **33** (2000) 6981–6991. Printed in the UK PII: S0305-4470(00)13283-4

An application of D-differentiation to solid-state physics*

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Received 13 April 2000, in final form 14 August 2000

Abstract. The operation of D-differentiation, introduced by Hurley and Vandyck (Hurley D and Vandyck M 1999 submitted), and briefly summarized here, is applied to the treatment of the semiclassical motion of electrons in crystals. It is shown that the corresponding trajectories are remarkable geometrical curves, called *euthygrammes*, which generalize the geodesics of Riemannian manifolds.

1. Introduction

In previous articles [1,2], we introduced the new operation of *D-differentiation* of a tensor or a spinor field on a manifold, and we studied some of its properties. We are currently engaged in work that will show how D-differentiation provides insight into some areas of physics, and, in this paper, we shall investigate the semiclassical trajectories of electrons in a crystal. We shall establish that D-differentiation enables one to interpret these trajectories in a manner analogous to that employed in general relativity for the motion of test particles in a gravitational field, where the trajectories are geodesics in a Riemannian manifold [3]. On the other hand, as we shall see, electron trajectories in a crystal are remarkable curves, called *euthygrammes*, which generalize geodesics to D-differentiation.

In order to render this work reasonably self-contained, we shall briefly recall hereafter, in section 2, fundamental aspects of D-differentiation. Euthygrammes will then be defined and studied in section 3. Finally, in sections 4 and 5, we shall turn our attention to electrons in crystals.

2. Fundamental aspects of D-differentiation

D-differentiation is an operation which generalizes simultaneously Lie and covariant differentiation [1, 2]. It may act on tensor or spinor fields, but we shall henceforth restrict our attention to tensor fields.

By definition, D-differentiation preserves tensor rank, commutes with tensor contractions and is linear, in the sense that

$$D_X(T+U) = D_X T + D_X U \tag{2.1}$$

$$D_X(kT) = k D_X T \tag{2.2}$$

* Dedicated to our former Colleague, the late John Delaney.

0305-4470/00/396981+11$30.00

for all tensor fields T and U (of the same rank), all vector fields X and all constants k. It also satisfies the Leibniz rule

$$D_X(T \otimes U) = (D_X T) \otimes U + T \otimes (D_X U) \tag{2.3}$$

for all tensor fields T and U, and all vector fields X. Moreover, for compatibility with the action of a vector field X on a function f, which is a tensor of rank $(0, 0)$, one imposes the condition that

$$D_X f := X(f) = \mathrm{d}f\,(X). \tag{2.4}$$

These axioms determine the action of D-differentiation on a tensor field of arbitrary rank [1,4] in terms of its action on a basis $\{\vec{e}_{(i)}\}$ of the tangent space to the manifold $\mathcal{M}$ under consideration. This action is defined by

$$D_X \vec{e}_{(j)} := \Lambda^i{}_j(X)\vec{e}_{(i)} \tag{2.5}$$

for some functions $\Lambda^i{}_j(X)$. The D-derivative $D_X Y$ of a vector field Y along a vector field X then reads

$$D_X Y = D_X(Y^i \vec{e}_{(i)}) \tag{2.6}$$

$$= \{X(Y^i) + \Lambda^i{}_j(X) Y^j\}\vec{e}_{(i)}. \tag{2.7}$$

In practice, $\Lambda^i{}_j(X)$ is given in terms of the components X^k of X by

$$\Lambda^i{}_j(X) := \lambda^i{}_{jk}\, X^k - A^i{}_j{}^a{}_b\, \vec{e}_{(a)}(X^b) \tag{2.8}$$

where the $A^i{}_j{}^a{}_b$ are the components of a tensor field. On the other hand, the symbols $\lambda^i{}_{jk}$ do *not* constitute a tensor, but satisfy the transformation law

$$\lambda'^i_{jk} = M^i{}_a\, \lambda^a{}_{bc}\, N^b{}_j\, N^c{}_k - M^i{}_a\, N^b{}_j\, A^a{}_b{}^c{}_d\, \vec{e}_{(c)}(N^d{}_k) + M^i{}_a\, \vec{e}_{(c)}(N^a{}_j) N^c{}_k \tag{2.9}$$

under the change of basis

$$\vec{e}'_{(i)} = \vec{e}_{(j)} N^j{}_i \tag{2.10}$$

for a given matrix N, and its inverse M. Moreover, after insertion of (2.8) in (2.7), the explicit form for $D_X Y$ in terms of the components of X and Y becomes

$$D_X Y = \{X(Y^i) + \lambda^i{}_{jk} X^k Y^j - A^i{}_j{}^a{}_b Y^j \vec{e}_{(a)}(X^b)\}\vec{e}_{(i)}. \tag{2.11}$$

The couple $(\lambda^i{}_{jk}, A^i{}_j{}^a{}_b)$ characterizes each D-differentiation operator. For instance, Lie and covariant differentiation are obtained from (2.11) with the following choice of symbols:

$$(\lambda^i{}_{jk}, A^i{}_j{}^a{}_b) = (\Gamma^i{}_{jk}, 0) \qquad \text{for} \quad \text{covariant differentiation} \tag{2.12}$$

$$= (-D^i{}_{jk}, \delta^i{}_b\, \delta^a{}_j) \qquad \text{for} \quad \text{Lie differentiation} \tag{2.13}$$

in which $\Gamma^i{}_{jk}$ and $D^i{}_{jk}$ are the connection coefficients and the anholonomicity of the basis:

$$[\vec{e}_{(i)}, \vec{e}_{(j)}] = D^k{}_{ij}\, \vec{e}_{(k)}. \tag{2.14}$$

No further properties of D-differentiation are required for our subsequent investigations. We are going to establish, in the next section, how D-differentiation enables one to generalize the concept of a Riemannian geodesic.

3. Euthygrammes

In a Riemannian manifold, one may define a geodesic as a curve along which its tangent vector is parallel transported. More precisely, if Γ is a curve expressed in coordinates x^i by

$$\Gamma : t \mapsto x^i(t) \tag{3.1}$$

for a certain parameter t, and if τ denotes the tangent vector to Γ, namely

$$\tau := \frac{\mathrm{d}}{\mathrm{d}t} \tag{3.2}$$

then Γ is a geodesic iff

$$\nabla_\tau \tau = 0 \tag{3.3}$$

where ∇ denotes covariant differentiation. Equivalently, one may write

$$\tau(\tau^i) + \Gamma^i{}_{jk}\, \tau^j \tau^k = 0. \tag{3.4}$$

In the holonomic frame $\{\partial/\partial x^i\}$, the geodesic equation (3.4) becomes

$$\frac{\mathrm{d}^2 x^i}{\mathrm{d}t^2} + \Gamma^i{}_{jk}\, \frac{\mathrm{d}x^j}{\mathrm{d}t} \frac{\mathrm{d}x^k}{\mathrm{d}t} = 0. \tag{3.5}$$

By analogy with (3.3), we define a vector field V as being *euthygrammic* iff

$$D_V V = 0. \tag{3.6}$$

Moreover, a *euthygramme*† is an integral curve of a euthygrammic vector field.

As a result of the coordinate expression (2.11) of D-differentiation, the criterion (3.6) of euthygrammicity also reads

$$V(V^i) + \lambda^i{}_{jk}\, V^j V^k - A^i{}_j{}^a{}_b\, \vec{e}_{(a)}(V^b) V^j = 0 \tag{3.7}$$

which emphasizes the parallel with (3.4). When V^i has been determined by (3.7), euthygrammes are solutions of the system

$$\frac{\mathrm{d}x^i}{\mathrm{d}t} = V^i(x^1, \ldots, x^n). \tag{3.8}$$

It is important to note that, in order to define a euthygramme, it is *not* possible, in general, to imitate the definition (3.3) of a geodesic as

$$D_\tau \tau = 0. \tag{3.9}$$

To determine why (3.9) is not valid in general, let us expand it in a basis according to (2.11):

$$\tau(\tau^i) + \lambda^i{}_{jk}\, \tau^j \tau^k - A^i{}_j{}^a{}_b\, \vec{e}_{(a)}(\tau^b) \tau^j = 0. \tag{3.10}$$

Because the tangent vector τ is only defined along Γ, the components τ^b appearing in (3.10) are functions of the parameter t describing Γ, so the contribution $\vec{e}_{(a)}(\tau^b)$ is devoid of meaning (in general), unless the operator $A^i{}_j{}^a{}_b\, \vec{e}_{(a)}(\cdot)\tau^j$ happens to differentiate *purely* along Γ. In other words, (3.10) only makes sense if $A^i{}_j{}^a{}_b\, \vec{e}_{(a)} \tau^j$ is proportional to the tangent vector τ. Such is the case when

$$A^i{}_j{}^a{}_b\, \vec{e}_{(a)} \tau^j = \Psi^i{}_b \tau \tag{3.11}$$

for a certain $\Psi^i{}_b$, or, equivalently, when

$$A^i{}_j{}^a{}_b = \Psi^i{}_b\, \delta^a{}_j. \tag{3.12}$$

† This new term is the anglicization of the Greek word $\epsilon\upsilon\vartheta\upsilon\gamma\rho\alpha\mu\mu\omicron\nu$, used by Aristotle [5] to mean a *straight line*. Indeed, in our present context, a euthygramme is a straight line (in a generalized sense), as is a geodesic in a Riemannian manifold.

This kind of D-differentiation is referred to as being of the *particular type*, as opposed to being of the *general type*, when $A^i{}_j{}^a{}_b$ is arbitrary.

When (3.12) is satisfied, the equation of the euthygramme reads

$$0 = \tau(\tau^i) + \lambda^i{}_{jk}\,\tau^j\tau^k - \Psi^i{}_j\,\tau(\tau^j) \tag{3.13}$$

$$= (\delta^i{}_j - \Psi^i{}_j)\tau(\tau^j) + \lambda^i{}_{jk}\,\tau^j\tau^k. \tag{3.14}$$

In particular, in the holonomic frame $\{\partial/\partial x^i\}$, the euthygramme (3.14) becomes

$$(\delta^i{}_j - \Psi^i{}_j)\frac{\mathrm{d}^2x^j}{\mathrm{d}t^2} + \lambda^i{}_{jk}\frac{\mathrm{d}x^j}{\mathrm{d}t}\frac{\mathrm{d}x^k}{\mathrm{d}t} = 0 \tag{3.15}$$

which is a clear generalization of (3.5).

On the other hand, for D-differentiation of a more general type, there is no option but to define euthygrammes by the two-step definition (3.7), (3.8). The advantage of (3.15) over (3.7), (3.8) is that the former is a system of *ordinary* differential equations, whereas the latter involves *partial* differentiation. In the application that follows, however, we shall only need D-differentiation of the particular type, so the central role will be played by (3.15).

4. Application to electrons in crystals

When an electron moves in a crystal, it is subjected to two kinds of force: *internal* forces, arising from the crystalline lattice, and forces produced by the *external* fields in which the crystal may be residing. When the external forces F are treated as perturbations of the internal ones, it is possible to establish [6, 7] that, to first order in the perturbation, the semiclassical position $X(t)$ of the electron is given by the following generalization of Newton's second law:

$$\mu^A{}_B\,\ddot{X}^B = F^A \tag{4.1}$$

where $\mu^A{}_B$ is the effective-mass tensor of the electron. Henceforth, as in (4.1), we shall use capital letters and capital indices for quantities referring to Cartesian coordinates.

Quantum mechanics enables one to calculate [6, 7] the effective mass in terms of the energy functions of the electron in the crystal, in the absence of the perturbation. The determination of $\mu^A{}_B$, however, does not concern us here. We are rather going to establish that (4.1) is a euthygramme of an operator of D-differentiation to be obtained. We shall see, in particular, that the effective mass is enciphered in the tensor $\Psi^i{}_j$ appearing in (3.15), and that the transformation law (2.9) for $\lambda^i{}_{jk}$ is satisfied.

To this end, let us begin by expressing (4.1) in curvilinear coordinates x^i, so as to make $\lambda^i{}_{jk}$ appear. Let us perform the change of variables

$$X^A := \xi^A(x^i) \tag{4.2}$$

for known functions ξ^A. (All quantities referring to curvilinear coordinates will be written with lower-case letters.) The velocity $\dot{X}^A$ becomes thus

$$\dot{X}^A := J^A{}_j\,\dot{x}^j \tag{4.3}$$

in which J denotes the Jacobian matrix of the coordinate transformation:

$$J^A{}_j := \frac{\partial\xi^A}{\partial x^j} := \xi^A_{,j}. \tag{4.4}$$

The inverse Jacobian matrix K relates then the Cartesian holonomic frame $\{\partial/\partial X^A\}$ to the curvilinear holonomic frame $\{\partial/\partial x^i\}$ by

$$\frac{\partial}{\partial X^A} = \frac{\partial x^i}{\partial X^A}\frac{\partial}{\partial x^i} := K^i{}_A\,\frac{\partial}{\partial x^i} \qquad KJ = I. \tag{4.5}$$

Moreover, after differentiating (4.3) with respect to the time, one finds

$$\ddot{X}^A = J^A{}_j\,\ddot{x}^j + J^A{}_{j,k}\,\dot{x}^k\dot{x}^j. \tag{4.6}$$

Therefore, the generalized version of Newton's second law becomes

$$F^A = \mu^A{}_B(J^B{}_j\,\ddot{x}^j + J^B{}_{j,k}\,\dot{x}^j\dot{x}^k) \tag{4.7}$$

which implies, after multiplying by $K^i{}_A$,

$$f^i := K^i{}_A\,F^A \tag{4.8}$$

$$= K^i{}_A\,\mu^A{}_B(J^B{}_j\,\ddot{x}^j + J^B{}_{j,k}\,\dot{x}^j\dot{x}^k). \tag{4.9}$$

To simplify the right-hand side of (4.9), let us rewrite $\mu^A{}_B$ differently:

$$\begin{aligned}\mu^A{}_B &= \mu^A{}_C\,\delta^C{}_B \\ &= \mu^A{}_C\,J^C{}_l\,K^l{}_B\end{aligned} \tag{4.10}$$

to obtain

$$\begin{aligned}f^i &= K^i{}_A\,\mu^A{}_C\,J^C{}_l(K^l{}_B\,J^B{}_j\,\ddot{x}^j + K^l{}_B\,J^B{}_{j,k}\,\dot{x}^j\dot{x}^k) \\ &= K^i{}_A\,\mu^A{}_C\,J^C{}_l(\ddot{x}^l + K^l{}_B\,J^B{}_{j,k}\,\dot{x}^j\dot{x}^k) \\ &= \mu^i{}_l(\ddot{x}^l + K^l{}_B\,J^B{}_{j,k}\,\dot{x}^j\dot{x}^k)\end{aligned} \tag{4.11}$$

where the transformation law for tensor indices has been exploited, in the form

$$\mu^i{}_l = K^i{}_A\,\mu^A{}_C\,J^C{}_l. \tag{4.12}$$

It follows from (4.11) that the equation of motion (4.1) becomes

$$f^i = m[(\delta^i{}_l - \Psi^i{}_l)\ddot{x}^l + \lambda^i{}_{jk}\,\dot{x}^j\dot{x}^k] \tag{4.13}$$

where m is a constant (representing a mass scale), provided the quantities $\Psi^i{}_j$ and $\lambda^i{}_{jk}$ are identified as

$$m(\delta^i{}_j - \Psi^i{}_j) := \mu^i{}_j = K^i{}_A\,\mu^A{}_C\,J^C{}_j \tag{4.14}$$

$$\lambda^i{}_{jk} := (\delta^i{}_l - \Psi^i{}_l)K^l{}_B\,J^B{}_{j,k}. \tag{4.15}$$

The relationship (4.14) may be inverted to isolate $\Psi^i{}_j$ as being

$$\Psi^i{}_j = \delta^i{}_j - \frac{1}{m}\mu^i{}_j. \tag{4.16}$$

Furthermore, after comparing (4.13) with the equation (3.15) of a particular type of euthygramme, one sees that the generalized version (4.1), (4.13) of Newton's second law may equivalently be written

$$m\,D_\tau\tau = f \tag{4.17}$$

where τ is the tangent vector to the trajectory. In (4.17), the operator of D-differentiation is characterized by the coefficients $\lambda^i{}_{jk}$ of (4.15), (4.16) and the quantities $A^i{}_j{}^a{}_b$ given by

$$A^i{}_j{}^a{}_b = \delta^a{}_j\,\Psi^i{}_b \tag{4.18}$$

$$= \delta^a{}_j\left(\delta^i{}_b - \frac{1}{m}\mu^i{}_b\right). \tag{4.19}$$

We have thus managed to interpret geometrically the motion of electrons in a crystal: in the absence of any external perturbation, electrons follow a euthygramme; on the other hand, perturbative forces cause the trajectory to deviate from a euthygramme, in accordance with (4.17).

Note that, by virtue of (2.12), (2.13), (4.19), the value of the tensor $A^{i}{}_{j}{}^{a}{}_{b}$ corresponds neither to that describing Lie differentiation, nor to that describing covariant differentiation, in general. This means that we have here a genuine example where neither Lie differentiation nor covariant differentiation suffices, in general, to provide a geometrical interpretation of the motion. Of course, if $\mu^{i}{}_{j} = m\delta^{i}{}_{j}$, the generalized law (4.1) is identical with Newton's original second law

$$m\ddot{X}^{A} = F^{A}. \tag{4.20}$$

In this very special case, the tensor $A^{i}{}_{j}{}^{a}{}_{b}$ of (4.19) vanishes, which indicates that the corresponding operator of D-differentiation does reduce to covariant differentiation. Such had to be the case, because it is well known [8] that Newton's second law (4.20) may be written

$$m\nabla_{\tau}\tau = f \tag{4.21}$$

in terms of covariant differentiation.

At this stage, it is important to recall that, whenever a set of coefficients $\lambda^{i}{}_{jk}$ has been prescribed, it must be ascertained that the transformation rule (2.9) is satisfied. With our present notation, the transformation matrix relating the bases $\{\partial/\partial X^{A}\}$ and $\{\partial/\partial x^{i}\}$ is the inverse Jacobian matrix K, as in (4.5), so that the transformation rule (2.9) reads

$$\lambda^{i}{}_{jk} = K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - K^{i}{}_{A}\,J^{B}{}_{j}\,A^{A}{}_{B}{}^{C}{}_{D}\,\frac{\partial J^{D}{}_{k}}{\partial X^{C}} + K^{i}{}_{A}\,\frac{\partial J^{A}{}_{j}}{\partial X^{C}}J^{C}{}_{k} \tag{4.22}$$

which the special form (4.18) for $A^{A}{}_{B}{}^{C}{}_{D}$ enables one to simplify as

$$\begin{aligned}\lambda^{i}{}_{jk} &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - K^{i}{}_{A}\,J^{B}{}_{j}\,\delta^{C}{}_{B}\,\Psi^{A}{}_{D}\,\frac{\partial J^{D}{}_{k}}{\partial X^{C}} + K^{i}{}_{A}\,\frac{\partial J^{A}{}_{j}}{\partial X^{C}}J^{C}{}_{k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - K^{i}{}_{A}\,J^{B}{}_{j}\,\Psi^{A}{}_{D}\,\frac{\partial J^{D}{}_{k}}{\partial X^{B}} + K^{i}{}_{A}\,\frac{\partial J^{A}{}_{j}}{\partial X^{C}}J^{C}{}_{k}.\end{aligned} \tag{4.23}$$

By virtue of the chain rule, all the derivatives appearing in (4.23) may be expressed in terms of the new variables x^{i}, to yield

$$\begin{aligned}\lambda^{i}{}_{jk} &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - K^{i}{}_{A}\,J^{B}{}_{j}\,\Psi^{A}{}_{D}(K^{l}{}_{B}\,J^{D}{}_{k,l}) + K^{i}{}_{A}(K^{l}{}_{C}\,J^{A}{}_{j,l})J^{C}{}_{k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - K^{i}{}_{A}\,\Psi^{A}{}_{D}\,J^{D}{}_{k,j} + K^{i}{}_{A}\,J^{A}{}_{j,k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - K^{i}{}_{B}\,\Psi^{B}{}_{A}\,J^{A}{}_{k,j} + K^{i}{}_{A}\,J^{A}{}_{j,k}.\end{aligned} \tag{4.24}$$

To simplify this expression, recall that $J^{A}{}_{k,j} = J^{A}{}_{j,k}$, and then, by elementary algebraic manipulations, obtain

$$\begin{aligned}\lambda^{i}{}_{jk} &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}J^{C}{}_{k} - (K^{i}{}_{B}\,\Psi^{B}{}_{A} - K^{i}{}_{A})J^{A}{}_{j,k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - (K^{i}{}_{B}\,\Psi^{B}{}_{C}\,\delta^{C}{}_{A} - \delta^{i}{}_{l}\,K^{l}{}_{A})J^{A}{}_{j,k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - (K^{i}{}_{B}\,\Psi^{B}{}_{C}\,J^{C}{}_{l}\,K^{l}{}_{A} - \delta^{i}{}_{l}\,K^{l}{}_{A})J^{A}{}_{j,k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} - (K^{i}{}_{B}\,\Psi^{B}{}_{C}\,J^{C}{}_{l} - \delta^{i}{}_{l})K^{l}{}_{A}\,J^{A}{}_{j,k}\\ &= K^{i}{}_{A}\,\lambda^{A}{}_{BC}\,J^{B}{}_{j}\,J^{C}{}_{k} + (\delta^{i}{}_{l} - \Psi^{i}{}_{l})K^{l}{}_{A}\,J^{A}{}_{j,k}.\end{aligned} \tag{4.25}$$

When the final form (4.25) is compared to the prescription (4.15), one sees that the transformation rule (2.9) is satisfied iff

$$\lambda^{A}{}_{BC} = 0 \tag{4.26}$$

and $\lambda^{i}{}_{jk}$ is calculated by (4.15).

The conclusion that we have reached is thus that all our formalism is self-consistent, and that the analogy with covariant differentiation is perfect: for Cartesian coordinates, the

coefficients $\lambda^A{}_{BC}$ vanish, just as the Christoffel symbols do for covariant differentiation. Furthermore, for curvilinear coordinates, the coefficients $\lambda^i{}_{jk}$ are given by (4.15), and it is not very difficult to prove that (4.15) contains the Christoffel symbols in the special case $\Psi^i{}_j = 0$.

Remark. The proper geometrical interpretation of the equation of motion (4.1) has been established in detail above, using D-differentiation. It is possible, however, *at the price of losing the geometrical interpretation of some of the framework*, to provide a different geometrization of (4.1), which does *not* employ general D-differentiation, but only *covariant* differentiation.

More precisely, one can show that (4.1) is equivalent to

$$\nabla_\tau \tau = a \tag{4.27}$$

where a is defined by

$$a^i := \nu^i{}_j \, f^j \qquad \nu^i{}_k \, \mu^k{}_j := \delta^i{}_j \tag{4.28}$$

and f^i is as in (4.8). The covariant derivative appearing in (4.27) must be calculated *via* the Christoffel symbols of the *fictitious* metric $g^\dagger_{ij}$ given by

$$g^\dagger_{ij} := \frac{\mu_{AB}}{m} J^A{}_i \, J^B{}_j \tag{4.29}$$

where m is a constant representing a mass scale. The metric $g^\dagger_{ij}$ has no geometrical significance: it constitutes a purely artificial concoction to recast (4.1) in the coordinate-independent language (4.27), using *only* covariant differentiation.

Establishing this assertion is not of much significance for our purposes. Therefore, only a few brief comments will suffice.

One begins by evaluating the Christoffel symbols $[ijk]^\dagger$ of the first kind for $g^\dagger_{ij}$ as being

$$[ijk]^\dagger = \frac{\mu_{AB}}{m} J^A{}_i \, J^B{}_{j,k} \tag{4.30}$$

with the notation of (4.4). A dagger has been attached to these Christoffel symbols to recall that they correspond to the fictitious metric $g^\dagger_{ij}$. Then, one defines the inverse metric $g^{\dagger ij}$ by

$$g^{\dagger ij} := m \nu^{PQ} \, K^i{}_P \, K^j{}_Q \qquad \nu^{PA} \, \mu_{AQ} = \delta^P{}_Q \tag{4.31}$$

and one employs this result to express the Christoffel symbols of the second kind for $g^\dagger_{ij}$ in the form

$$\{{}^i_{jk}\}^\dagger := g^{\dagger ia} [ajk]^\dagger = K^i{}_A \, J^A{}_{j,k}. \tag{4.32}$$

The combination of (4.27) with (4.32) yields an equation that is equivalent to (4.11), thus proving (4.27).

Let us emphasize† that the formalism (4.27)–(4.29) is *not* the one that we recommend as a geometrical interpretation of the motion of electrons in crystals, but rather (4.17)–(4.19). This is because (4.27)–(4.29), albeit *mathematically* equivalent to (4.17)–(4.19), is based on a metric ($g^\dagger_{ij}$) lacking *physical* meaning. In other words, the *physical* metric of three-dimensional ambient space is the one required, when Schrödinger's equation is set up, to quantize the kinetic part of the Hamiltonian, whereas the formalism (4.27)–(4.29) involves the *fictitious* metric $g^\dagger_{ij}$.

On the other hand, the framework (4.17)–(4.19), which is based on D-differentiation, is *independent* of the metric. Indeed, *nowhere* does the metric appear in the component expression (2.11) for the D-derivative of a vector field. (D-differentiation is thus purely

† The authors would like to thank the referee, who pointed out the desirability of insisting on this point.

affine.) Therefore, the framework (4.17)–(4.19) does not interfere with the metric structure of space, which retains its usual physical interpretation. In fact, we only mentioned the alternative formalism (4.27)–(4.29) for the sake of mathematical completeness, and we shall henceforth discard it.

At this stage, we have at our disposal the general theory of electrons in crystals. Given that the concept of D-differentiation may be unfamiliar to some readers, we are going to illustrate the general construction, in the next section, by applying the framework (4.17)–(4.19) to a well known 'text-book' problem, namely the motion of an electron in a particular crystal subjected to a uniform magnetic field.

5. Simple illustration

Following [7], we shall consider the motion of an electron of charge q in the neighbourhood of the conduction-band edge point of either a silicon or a germanium crystal. The reader is referred to [7] for physical details.

In accordance with [7], we shall assume that the energy surfaces $\epsilon_n(k)$ generated by the crystal, for a wave of wavevector k, are ellipsoids of revolution. By an appropriate choice of the Cartesian axes $\{\partial/\partial X^A\}$, one may thus write [7]

$$2\hbar^{-2}\epsilon_n(k) = (k_1^2 + k_2^2)/m_{\mathrm{t}} + k_3^2/m_{\mathrm{l}} \tag{5.1}$$

in which m_{t} and m_{l} are two parameters, interpreted as the 'transversal mass', and the 'longitudinal mass', respectively.

Furthermore, the laws of quantum mechanics [6, 7] imply that the inverse effective mass $(1/\mu)^{AB}$ is related to the energy surfaces by

$$(1/\mu)^{AB} = \frac{1}{\hbar^2}\frac{\partial^2\epsilon_n}{\partial k_A \partial k_B}. \tag{5.2}$$

In the particular case of (5.1), a simple calculation yields then

$$\mu^A{}_B = \begin{pmatrix} m_{\mathrm{t}} & 0 & 0 \\ 0 & m_{\mathrm{t}} & 0 \\ 0 & 0 & m_{\mathrm{l}} \end{pmatrix}. \tag{5.3}$$

In addition, the crystal is subjected to an external magnetic field B of the form

$$B = \beta\left(\sin\alpha\frac{\partial}{\partial X^1} + \cos\alpha\frac{\partial}{\partial X^3}\right) \tag{5.4}$$

where the constant β is the magnitude of the field, and α denotes the angle between the field and the third axis. The *external* force F experienced by the electron moving in the crystal with a velocity V is therefore given by the Lorentz force

$$F = \frac{q}{c}V \times B \tag{5.5}$$

in the Gaussian units employed in [7].

In order to apply the geometrical framework (4.17)–(4.19), we firstly note that the coordinates that we have selected are Cartesian, so that the lower-case coordinates x and the upper-case coordinates X, introduced in (4.2), coincide. Consequently, the Jacobian matrix $J^A{}_j$ of (4.4) is trivial:

$$J^A{}_j = \delta^A{}_j. \tag{5.6}$$

This information, combined with (5.3) and the definition (4.12), (4.19), yields the quantities $A^{i}{}_{j}{}^{k}{}_{l}$ as being

$$A^{\bullet}{}_{B}{}^{C}{}_{\bullet} = \delta^{C}{}_{B}\begin{pmatrix} 1-m_{\mathrm{t}}/m & 0 & 0 \\ 0 & 1-m_{\mathrm{t}}/m & 0 \\ 0 & 0 & 1-m_{\mathrm{l}}/m \end{pmatrix} \tag{5.7}$$

where the entries indicated on the left-hand side by dots refer to the row index and the column index of the matrix on the right-hand side.

The next element required to evaluate the operator of D-differentiation is the set of coefficients $\lambda^{A}{}_{BC}$. By virtue of (4.26), all these coefficients vanish, because the coordinates are Cartesian.

Moreover, let τ denote the tangent to the trajectory $X^{A}(t)$ of the electron. (It is physically interpreted as the velocity of this electron.) One has thus

$$\tau = \frac{\mathrm{d}}{\mathrm{d}t} = \dot{X}^{A}\frac{\partial}{\partial X^{A}}. \tag{5.8}$$

Consequently, when the component expansion (2.11) of D-differentiation is used (with the appropriate values for $\lambda^{A}{}_{BC}$ and $A^{\bullet}{}_{B}{}^{C}{}_{\bullet}$), the final result for the D-derivative $D_{\tau}\tau$ reads

$$D_{\tau}\tau = \frac{m_{\mathrm{t}}}{m}\left(\tau[\tau^{1}]\frac{\partial}{\partial X^{1}} + \tau[\tau^{2}]\frac{\partial}{\partial X^{2}}\right) + \frac{m_{\mathrm{l}}}{m}\tau[\tau^{3}]\frac{\partial}{\partial X^{3}} \tag{5.9}$$

$$= \frac{m_{\mathrm{t}}}{m}\left(\ddot{X}^{1}\frac{\partial}{\partial X^{1}} + \ddot{X}^{2}\frac{\partial}{\partial X^{2}}\right) + \frac{m_{\mathrm{l}}}{m}\ddot{X}^{3}\frac{\partial}{\partial X^{3}}. \tag{5.10}$$

Finally, after an elementary calculation based on (5.4), (5.5), one finds, for the external force F, the expression

$$F = (q\beta/c)\left[(\dot{X}^{2}\cos\alpha)\frac{\partial}{\partial X^{1}} + (\dot{X}^{3}\sin\alpha - \dot{X}^{1}\cos\alpha)\frac{\partial}{\partial X^{2}} - (\dot{X}^{2}\sin\alpha)\frac{\partial}{\partial X^{3}}\right] \tag{5.11}$$

which enables one to formulate the equation of motion (4.17), in matrix language, as

$$\begin{bmatrix} m_{\mathrm{t}} & 0 & 0 \\ 0 & m_{\mathrm{t}} & 0 \\ 0 & 0 & m_{\mathrm{l}} \end{bmatrix}\begin{bmatrix} \ddot{X}^{1} \\ \ddot{X}^{2} \\ \ddot{X}^{3} \end{bmatrix} = (q\beta/c)\begin{bmatrix} \dot{X}^{2}\cos\alpha \\ \dot{X}^{3}\sin\alpha - \dot{X}^{1}\cos\alpha \\ -\dot{X}^{2}\sin\alpha \end{bmatrix}. \tag{5.12}$$

This is a linear system of ordinary differential equations for $X^{A}(t)$.

There is no difficulty in proving that (5.12) admits a solution of the kind

$$\dot{X}^{A} = K^{A}\mathrm{e}^{\mathrm{i}\omega t} \tag{5.13}$$

for certain (non-vanishing) constants K^{A} and ω, provided ω reads

$$\omega = (q\beta/c)\left[\frac{\sin^{2}\alpha}{m_{\mathrm{t}}m_{\mathrm{l}}} + \frac{\cos^{2}\alpha}{m_{\mathrm{t}}^{2}}\right]^{1/2}. \tag{5.14}$$

In the context of *Solid-State Physics*, ω is interpreted [7] as the cyclotron resonant frequency, and the value (5.14) provided by our geometrical framework is identical with that stated in [7], as it should be.

It should be noted that the above treatment, based on Cartesian coordinates, is readily adapted to curvilinear coordinates, for instance cylindrical coordinates (r, θ, z). In this case, one would identify the coordinates X^{A} and x^{i} of (4.2) as

$$X^{1} = r\cos\theta \qquad X^{2} = r\sin\theta \qquad X^{3} = z \qquad X^{A} = (X, Y, Z) \qquad x^{i} = (r, \theta, z) \tag{5.15}$$

and the Jacobian matrix $J^A{}_j$ would now become non-trivial.

The effective mass tensor, in curvilinear coordinates, would then be obtained from its Cartesian components $\mu^A{}_B$ by (4.12), whereas the quantities $A^{i\ k}_{j\ l}$ would be calculated via (4.19). The coefficients $\lambda^i{}_{jk}$ would be non-vanishing, and would follow from (4.15), (4.16). Finally, all this would be combined with the component expansion (2.11) of the operator of D-differentiation, to express the equation of motion (4.17), very much as we did above in Cartesian coordinates.

6. Conclusion

In this article, we have shown how D-differentiation sheds light on the motion of electrons in a crystal. This required introducing the concepts of a euthygrammic vector field and a euthygramme.

A vector field V was defined, in section 3, as being euthygrammic iff it is 'D-transported' along itself, in the sense that

$$D_V V = 0. \tag{6.1}$$

A euthygramme is then an integral curve of a euthygrammic vector field.

We also established that, when D-differentiation is characterized by a tensor field $A^{i\ a}_{j\ b}$ of the form

$$A^{i\ a}_{j\ b} = \Psi^i{}_b\, \delta^a{}_j \tag{6.2}$$

for a certain $\Psi^i{}_b$, the equation of a euthygramme with tangent vector τ may be expressed as

$$D_\tau \tau = 0 \tag{6.3}$$

which circumvents the need for considering euthygrammic vector fields to define euthygrammes. A more detailed study of euthygrammes will be provided in [9].

In section 4, we investigated the semiclassical motion of an electron in a crystal. We saw that the internal forces arising from the crystalline lattice are enciphered in the field $\Psi^i{}_b$ of (6.2), via the effective mass $\mu^i{}_b$ of the electron, as

$$A^{i\ a}_{j\ b} = \Psi^i{}_b\, \delta^a{}_j = \left(\delta^i{}_b - \frac{1}{m}\mu^i{}_b\right)\delta^a{}_j, \tag{6.4}$$

where m denotes a mass scale, for instance the mass of the electron (*in vacuo*).

In the presence of a perturbative external force f, the trajectory of an electron reads

$$m D_\tau \tau = f \tag{6.5}$$

in which the operator D is based on the coefficients $A^{i\ a}_{j\ b}$ of (6.4). Consequently, when no perturbation acts, the electron follows a euthygramme, whereas a perturbation causes the trajectory to deviate from that euthygramme, in accordance with (6.5).

We emphasized that the operator D constructed from (6.4) reduces neither to Lie differentiation nor to covariant differentiation, in general. The equation of motion (6.5) provides thus an example where neither Lie differentiation nor covariant differentiation suffices to produce a completely geometrical interpretation of the trajectory. Indeed, an alternative formulation was developed, which involved only *covariant* differentiation, but it required the introduction of the fictitious metric (4.29), which is devoid of direct geometrical meaning. (That alternative formulation was therefore eventually discarded.) An additional advantage of expressing the equation of motion (6.5) with D-differentiation is that (6.5) does not need *any* metric, so it is purely affine.

Of course, the results presented in this article do not, by any means, invalidate the traditional method [6, 7] for obtaining the trajectories of electrons in crystals by solving (4.1), just as (for instance) the possibility of re-interpreting Newton's second law as a geodesic in a Riemannian space does not invalidate the traditional equation $m\ddot{X} = F$. However, as classical mechanics, relativity and gauge theories have shown, being able to express a physical problem in geometrical terms often leads to further *conceptual* insight. Moreover, the laws of geometry may then sometimes be invoked to simplify even the *computational* aspects of the problem.

This feature is clearly exemplified, again, by the re-interpretation of $m\ddot{X} = F$ as a Riemannian geodesic: the former approach is only valid in an *inertial* frame, whereas the geometrical formulation, being based on the *coordinate-free* concept of a geodesic, holds in an *arbitrary* frame, which means that the geometrical method takes pseudo-forces *automatically* into account. Something similar may be said of our geometrical interpretation of the trajectories of electrons in crystals, where pseudo-forces are determined by the coefficients $\lambda^i{}_{jk}$.

Acknowledgments

It is a pleasure to thank Professor S Fahy and Dr P Delaney (National University of Ireland, Cork) for interesting discussions. The Dublin Institute for Advanced Studies is also gratefully acknowledged for library facilities provided during the completition of this work.

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